Co-Optimization of
Fuels & Engines

Co-Optima:
Gasoline Direct-Injection Sprays

Marco Arienti, Lyle M. Pickett, and Christopher F. Powell, Scott A. Skeen

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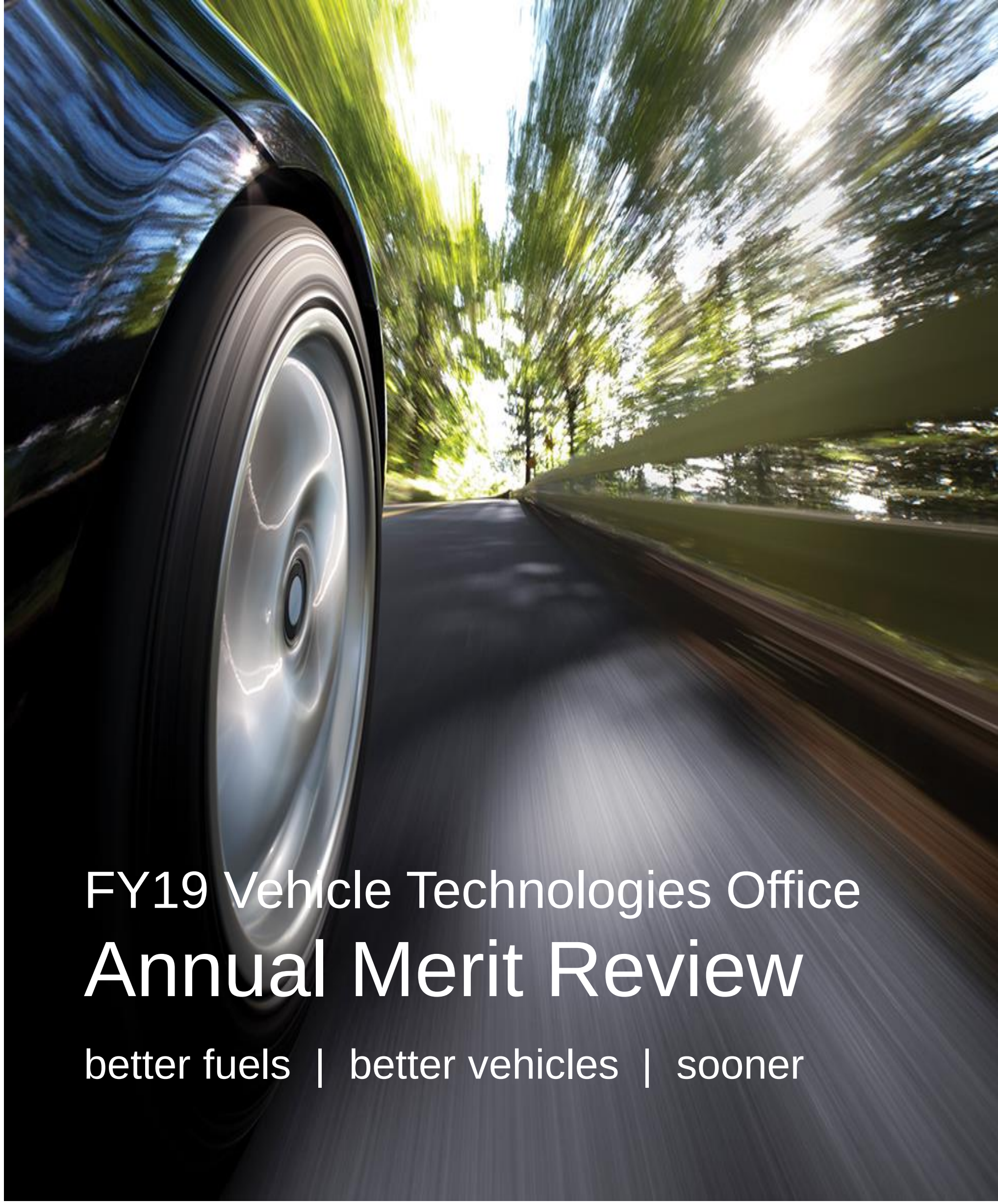
Project ID: FT074



Overview

Projects

Abbrev.	Description
OI	Optical Imaging (Pickett & Skeen)
XD	X-Ray Diagnostics (Powell)
SM	Simulation/Modeling (Arienti)

Barriers*

- Need improved combustion modes & understanding of fuel effects thereon
- Understanding direct-injection sprays as a key pathway towards high-efficiency engines (multimode and lean SI)
- CFD model improvement for engine design/optimization

*from https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf & https://www.energy.gov/eere/vehicles/advanced-combustion-strategies

Budget

Project	Lab	FY18 [$k]	FY19 [$k]
OI	Sandia	$250	$275
XD	Argonne	$150	$155
SM	Sandia	$190	$150

Timeline

Project	Start	End
OI	10/2015	9/2019
XD	10/2015	9/2019
SM	10/2017	9/2019

Relevance of fuel injection to advanced multimode combustion

Spray affects…

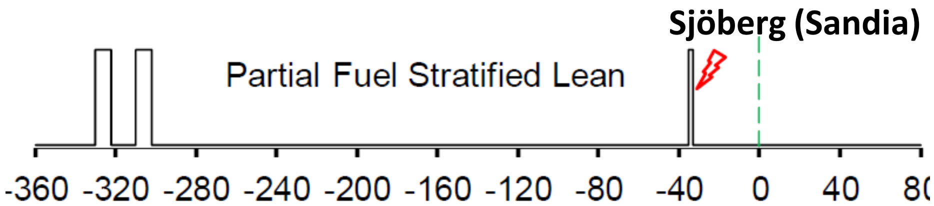
- liquid penetration, mixture preparation, and burn rate
- propensity to knock or auto-ignite in standard SI or multimode

Wall wetting or liquid in the bulk charge

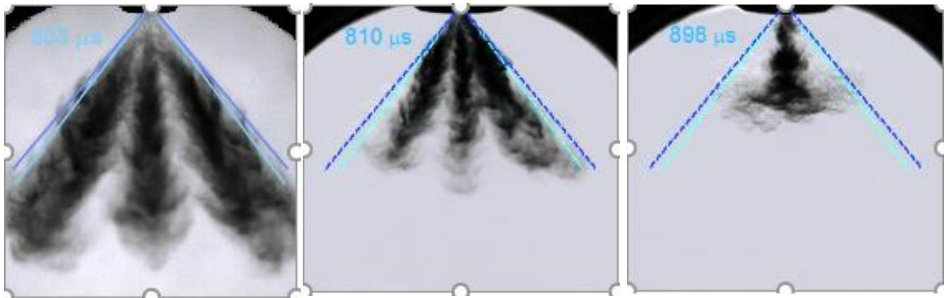
- creates fuel-rich, PM-forming combustion
- is not completely explained by fuel physical properties (distillation curve) or soot metrics (PMI index)

Conditions vary widely, significantly changing spray

Injection strategy for multimode combustion



Intake injection (ECN* G3 condition)	Late injection (ECN G condition)	Near-TDC injection (High T, P condition)



333 K, 1.0 kg/m3	573 K, 3.5 kg/m3	800 K, 9.0 kg/m3

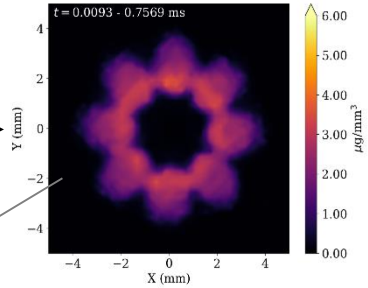
With intake T=333K, P=1.0bar, CR=12

CAD TDC	Temperature	Pressure	Density
intake open	333 K	1.0 bar	1.1 kg/m3
-52	511 K	5.2 bar	3.6 kg/m3
-19	711 K	18.7 bar	9.2 kg/m3

Approach

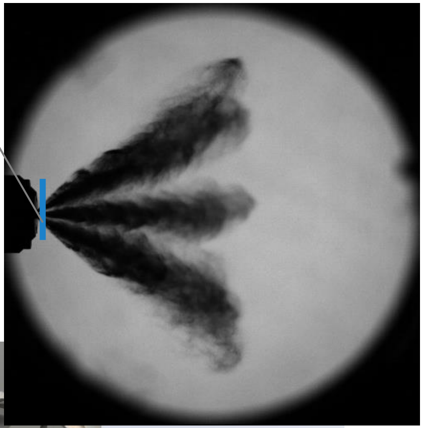
Quantitative fuel concentration by spray tomography

SX = X-Ray Diagnostics
(Powell, ANL)

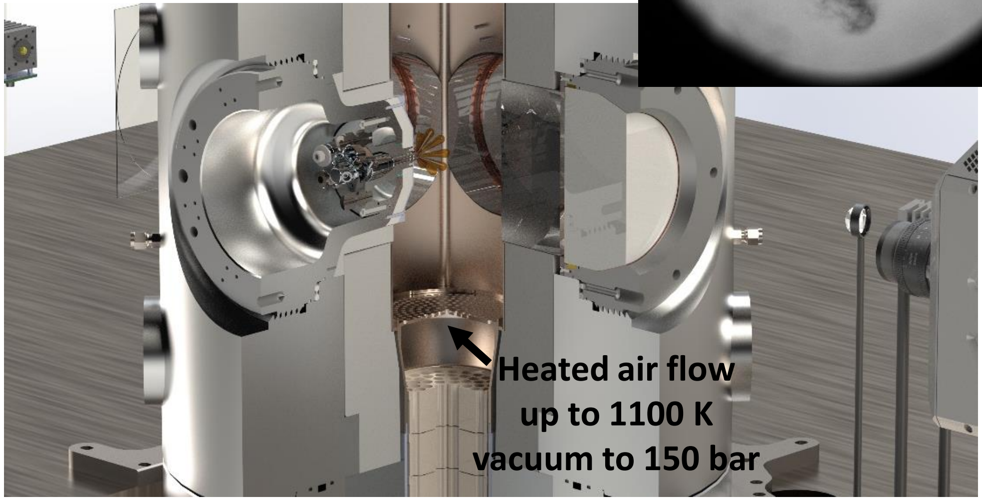


planes at z = 1-2 mm

Optical extinction imaging



OI = Optical Imaging
(Pickett, SNL)

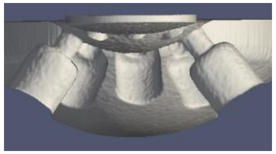


Use same fuels and injector (ECN Spray G)

8-hole, stepped

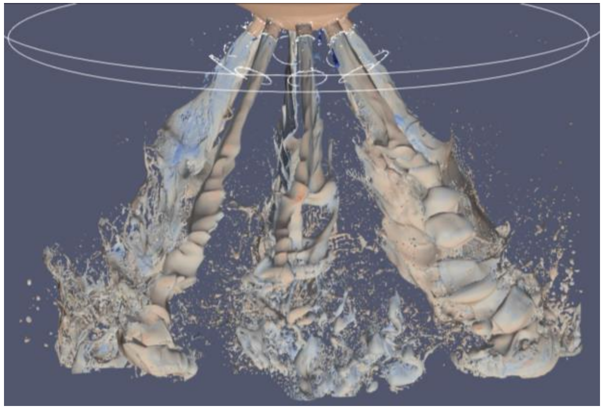
80° total angle

full geometry provided



geometry from xray tomography, Argonne

SM = Simulation / modeling
(Arienti, SNL)



Research using Tier 3-selected fuels

Fuels used throughout CoOptima program, including Sandia optical engine

	Refinery Stock					Surrogate Blends					
	Olefins	*Cyclo-alkanes*	*Alkyl-ate*	*E30*	*Arom-atic*	*Iso-butanol*	*Diisobu tylene*	*BOB4*	*Iso-Octane*	*E20*	*B20*
RON	98.2	97.8	98	97.9	98.1	98.1	98.3	90.3	100		
MON	88	86.9	96.7	87.1	87.6	88	88.5	84.7	100		
						41.7	44.2	55	100	80	80
T10 [°C]	77	56	93	61	59	11.4	12.1	15	0	0	0
T50 [°C]	104	87	100	74	108	19.0	20.1	25	0	0	0
T90 [°C]	136	143	106	155	158	3.8	4.0	5	0	0	0
TF [°C]	198	204	161	204	204	0	19.6	0	0	0	0
IsoButanol [Vol. %]	0	0	0	0	0	24.1	0	0	0	0	20
Ethanol [Vol. %]	0	0	0	30	0	0	0	0	0	20	0
Oxygenates [Vol. %]	0	0	0	30.6	0	24.1	0	0	0	20	20
Aromatics [Vol. %]	13.4	33.2	0	8.1	30.8	19	20.1	25	0	0	0
Olefins [Vol. %]	26.5	1.6	0	5	4.2	3.8	4	5	0	0	0
Paraffins [Vol. %]	56.4	40.6	100	57.1	65	53.1	56.3	70	100	80	80
Cycloalkanes [Vol. %]	2.9	24.2	0	7	8	0	0	0	0	0	0
Particulate Matter Index	1.00	1.54	0.22	1.28	1.80	0.40	0.47	0.48	0.19		
Net Heat of Combustion [MJ/kg]	44.1	43.2	44.5	38.2	43	40.6	43.5	43.3	44.3		
Stoichiometric Air-Fuel Ratio	14.8	14.5	15.1	12.8	14.5	13.8	14.7	14.6	15		
Heat of Vaporization [kJ/kg]	-	-	309	536	363	416	330	344	306		

Vol. %	**RON**	**BP [°C]**
iso-octane	**100**	**99.5**
n-heptane	**0**	**98**
toluene	**121**	**111**
1-hexene	**76**	**63.4**
diisobutylene	**106**	**107.9**
isobutanol	**105**	**101.4**
ethanol	**109**	**78.5**

BOB4 surrogate for base gasoline was developed by NREL, with full properties/tests available at https://fuelsdb.nrel.gov/fmi/webd/FuelEngineCoOptimization

Milestones

Mo/Yr	Proj.	Description of Milestone or Go/No-Go Decision	Status
Jan. ’19	OI	Quantify liquid plume penetration in 3D for Tier-3 selected RON98 fuels (>10 fuels) over a range of intake conditions	✓
Mar. ’19	OI	Demonstrate feasibility for mixed-mode ignition/flame imaging	✓
Aug. ’19	OI	Compare ignition characteristics for Tier-3 RON98 fuels	Pending
Mar. ’19	XD	Perform measurements of the near-nozzle fuel distribution resulting from iso-octane/ethanol/butanol blends under flash-boiling and non-flashing conditions	✓
Jul. ’19	XD	Measure near-nozzle droplet sizing using USAXS	Pending
Feb. ’19	SM	Simulate ECN Spray G mixing/breakup for two fuel blends	✓
Jun. ’19	SM	Implement improved relaxation model for flash-boiling conditions	Pending

OI = Optical Imaging (Pickett, SNL)

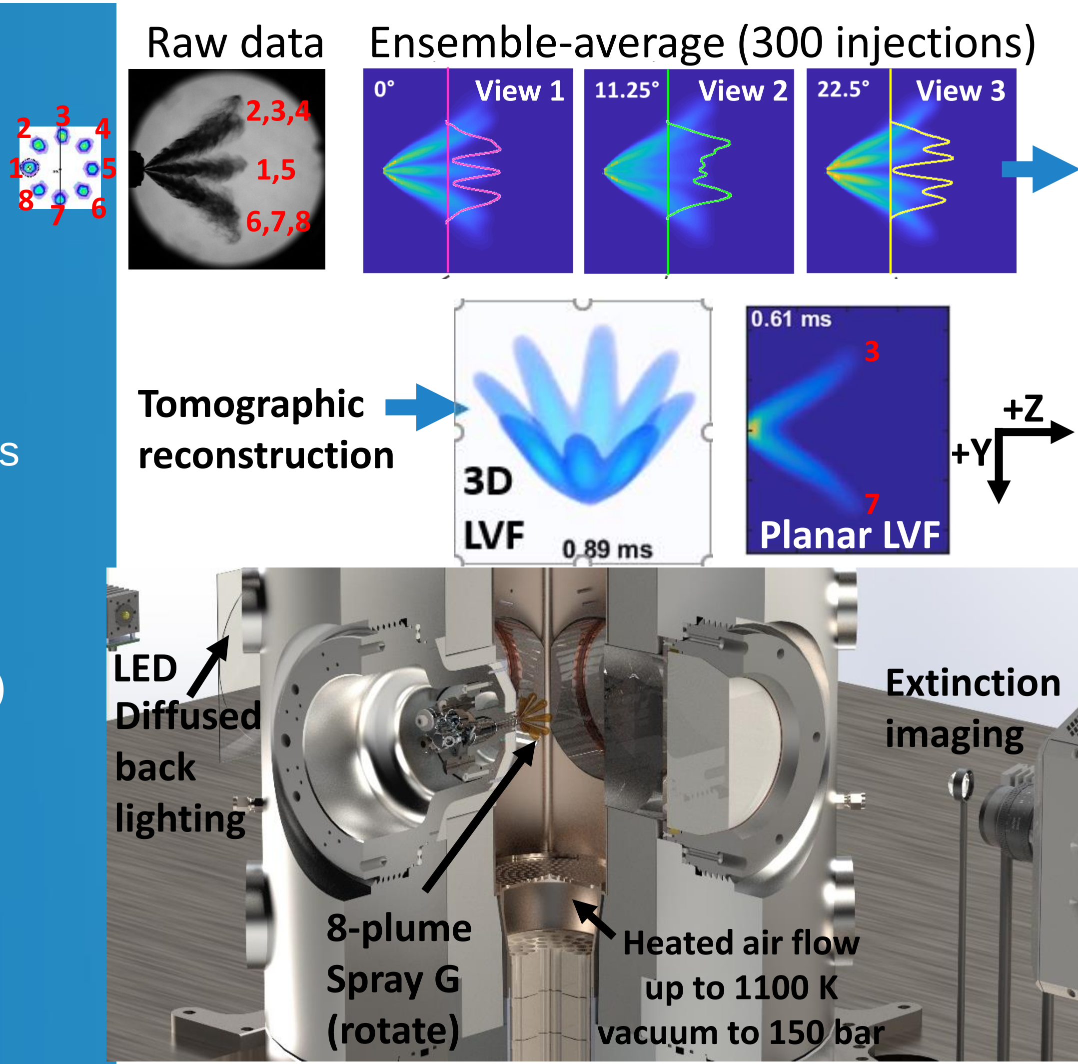
Developed diagnostic for 3D liquid volume fraction using high-throughput chamber

High-speed extinction tomography

- Provides DOWNSTREAM measurement of plume direction, a significant metric for wetting, mixing and CFD development
- Offers significant advantages compared to planar laser diagnostics
- Shows spatial position and timing of liquid vaporization

New flow spray facility offers

- Extensive optical access (>100 mm)
- Range of conditions to mimic intake or late-injection conditions, covering standard SI and multimode
- Throughput to generate massive ensemble-average datasets



OI = Optical Imaging (Pickett, SNL)

Light distillate components encourage spray collapse

Even using heated fuel and limited injection (10 mg), there is substantial liquid penetration

- reference engine: bore/stroke 86/95 mm
- E30 has both high BP and high latent HoV

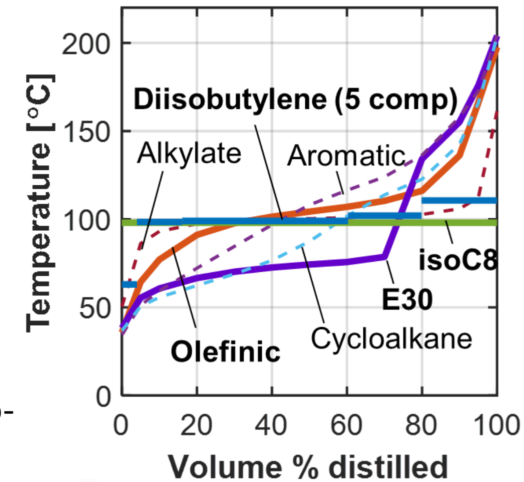
Small levels of light distillate are important

- Collapsed sprays do not mix well and likely impinge upon piston
- Olefinic blend affected with <20% light dist.

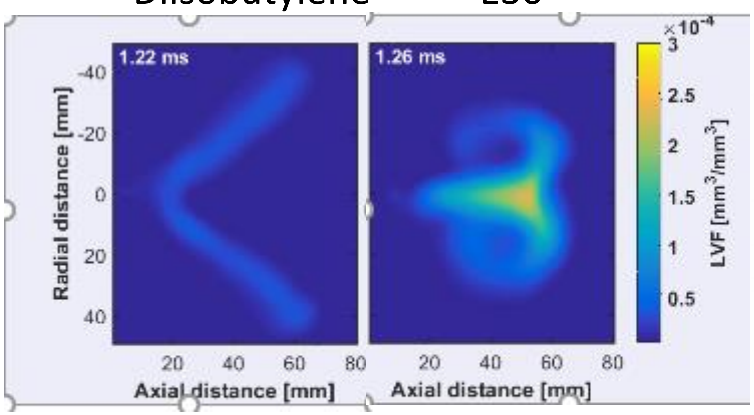
Impact on fuel selection:

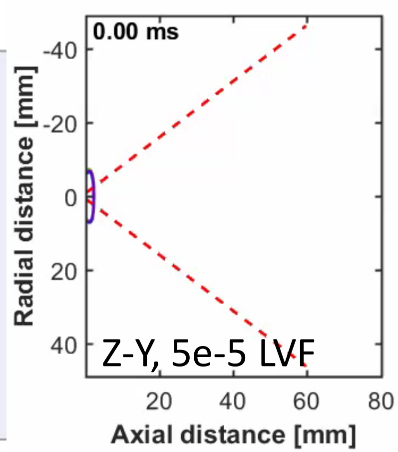
- Light distillate fraction needs consideration, in concert with spray strategy
- Wide-angle injectors and short, multiple injections may be needed

ECN "G2" intake-injection condition
8-hole, 80° injector
T_{inj} = 90° C
P_{inj} = 200 bar
t_{inj} = 0.78 ms, 10 mg
P_{gas} = 0.5 bar
T_{gas} = 60° C
flash boiling with iso-octane $P_{vap} > P_{gas}$



Diisobutylene E30

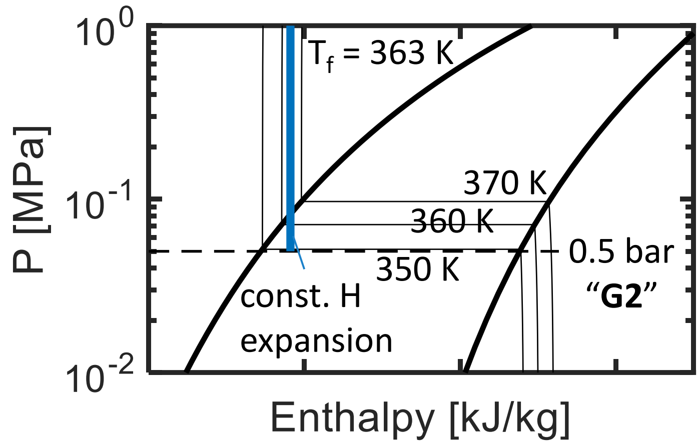




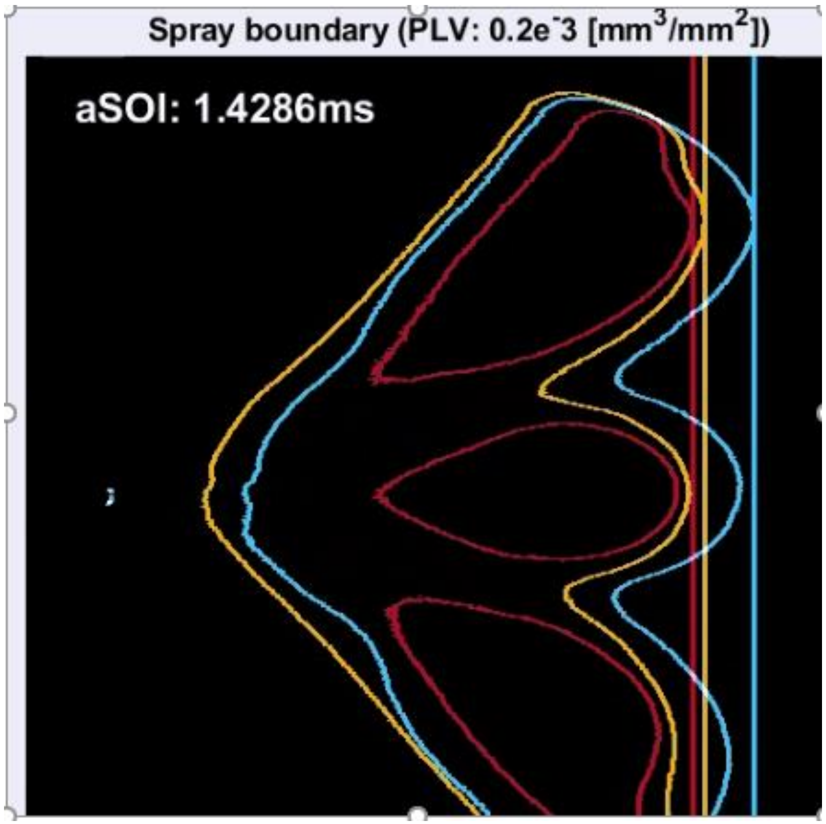
Z-Y plane LVF

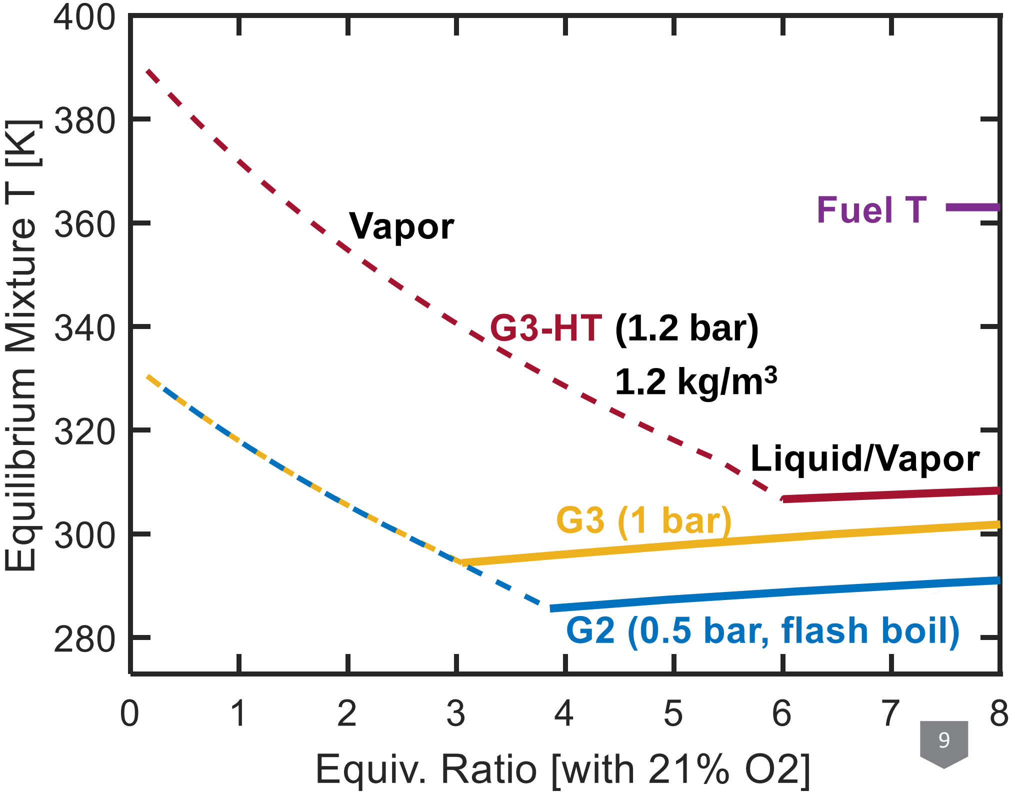
OI = Optical Imaging (Pickett, SNL)

Flash-boiling conditions do not necessarily undergo immediate evaporation



Liquid boundary based upon "projected liquid volume" along a line of sight





OI = Optical Imaging (Pickett, SNL)

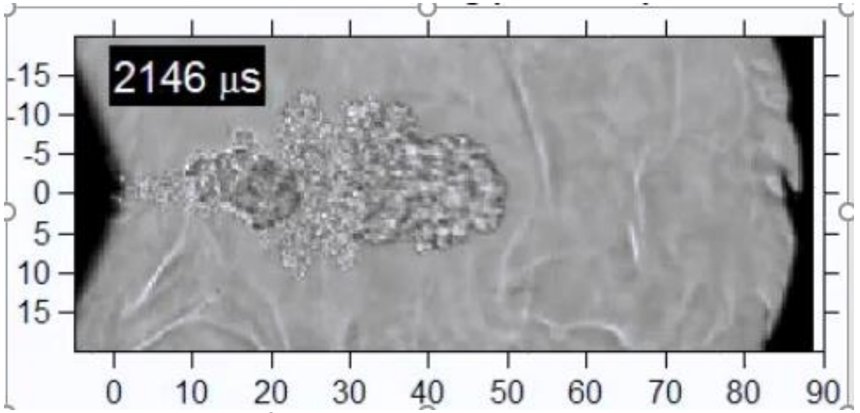
Imaging reveals both ignition and flame propagation at multimode conditions

Late-compression gasoline injection

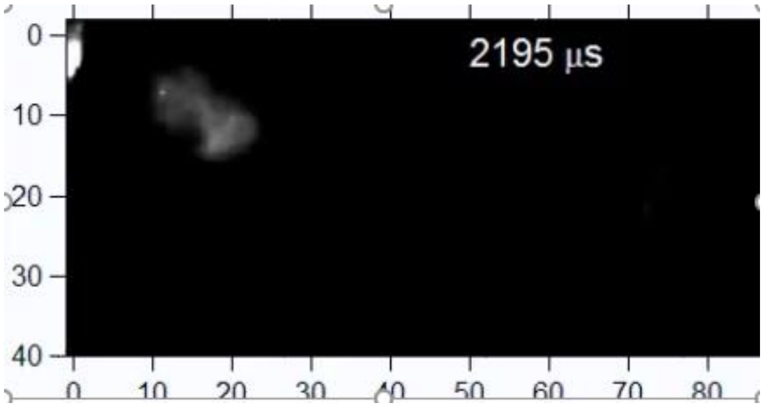
- highly stratified mixture with no "background" air/fuel mixture
- autoignition of "first-injected" fuel in wake of head vortex
- apparent flame propagation through much of the charge
- autoignition sites noticeable as well
- >20 m/s convection of flame
- non-sooting combustion

<u>Ambient gas</u>
T_a = 1050 K, P = 19 bar
21% oxygen (air)
<u>fuel</u>
iso-octane
100 bar
~2.7 mg injection

Schlieren imaging (side view)

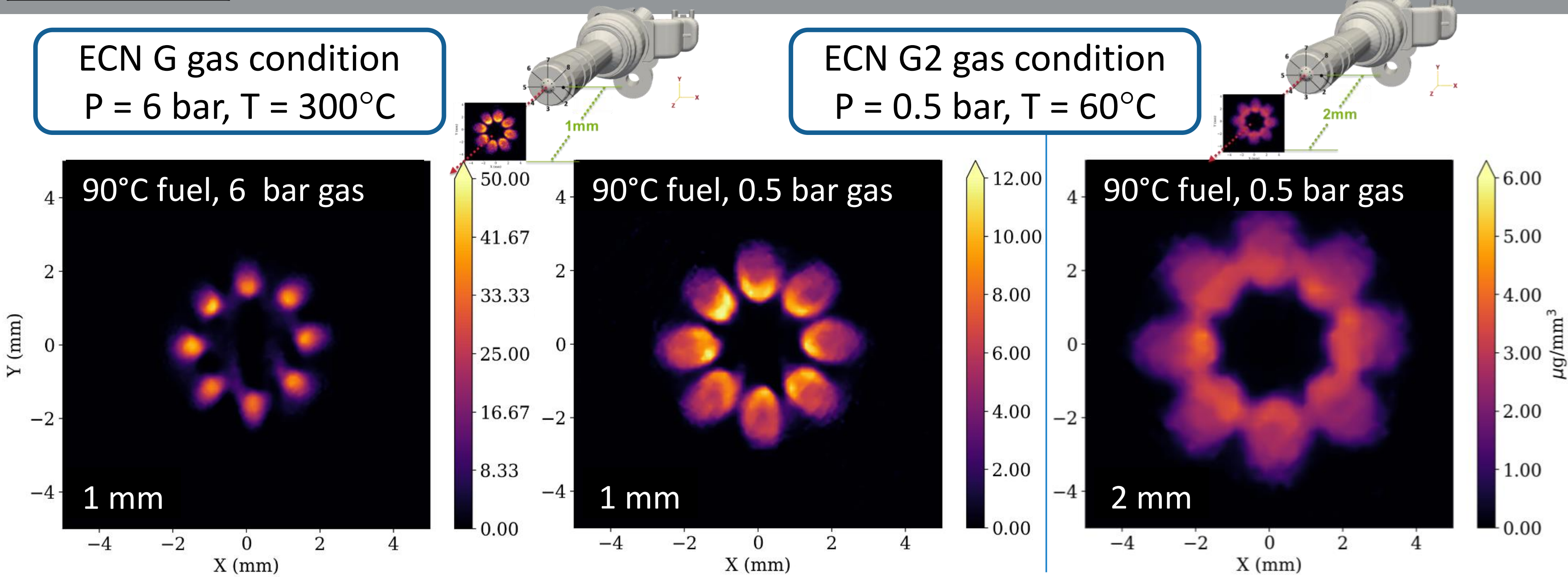


Mie-scatter/chemiluminescence (bottom view)



XD = X-Ray Diagnostics (Powell, ANL)

Measurements of the near-nozzle fuel distribution in flash-boiling sprays

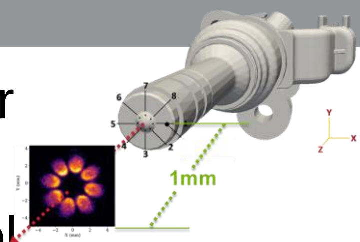


2D slices obtained using x-ray tomography showing the iso-octane density under non-vaporizing and flash-boiling conditions

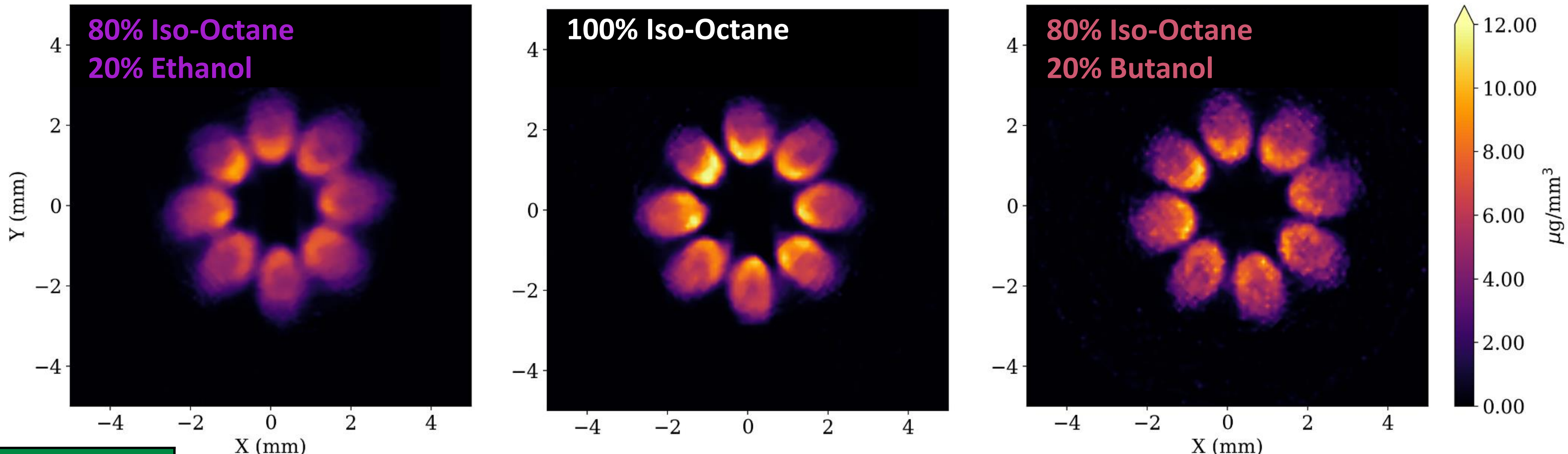
- Liquid fuel density has been quantified at 1 - 2 mm downstream of the injector for three different fuel blends
- As expected, spray plumes are more diffuse under flash-boiling cond's
- Simulations (submitted at ECN6 workshop) underpredicted the measured dispersion, suggesting a need for modeling research at these conditions

XD = X-Ray Diagnostics (Powell, ANL)

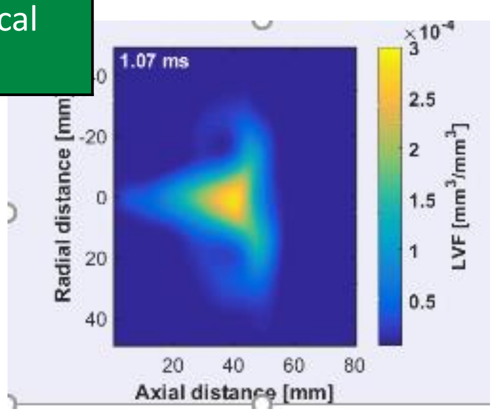
Fuel effect on flash-boiling Spray G2

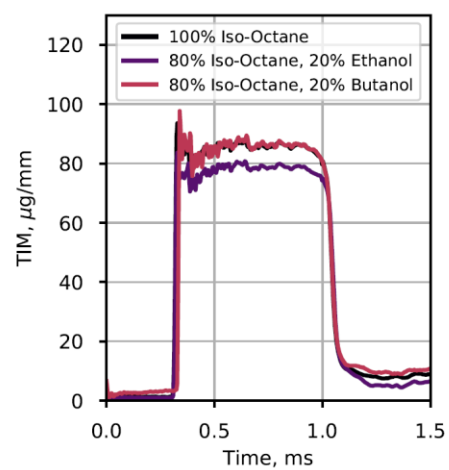


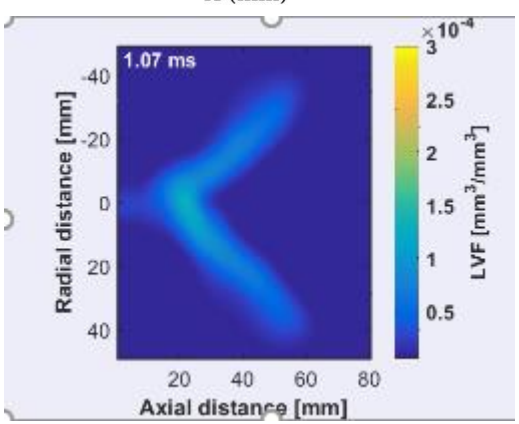
- Near-nozzle measurements show stronger plume growth for ethanol mixture, particularly for flash-boiling conditions
- Measured cross-sectional mass (TIM) decreases for ethanol



OI = Optical Imaging







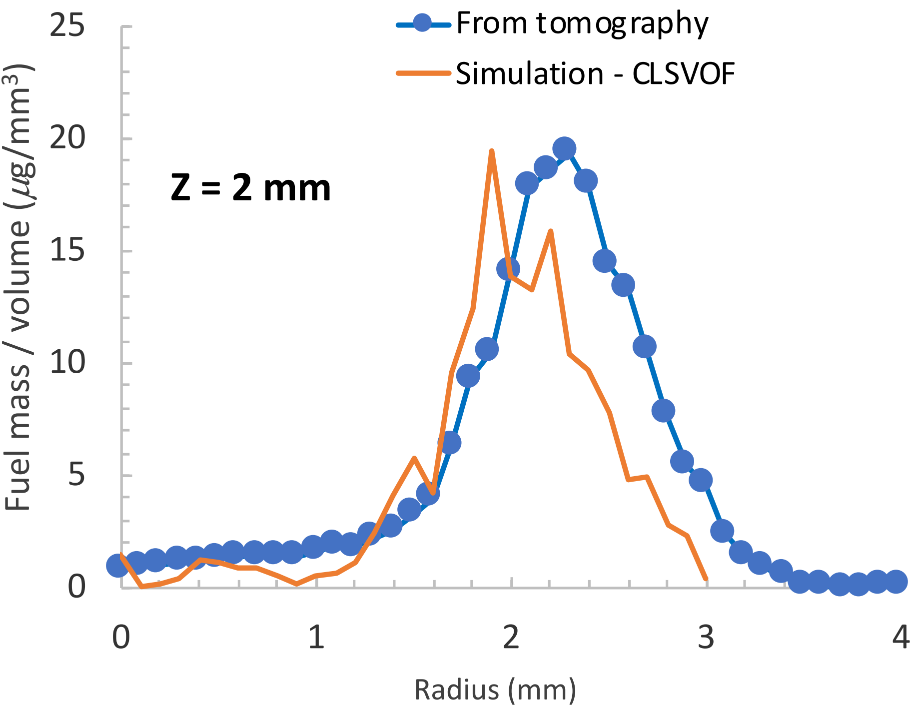
Z-Y plane LVF

SM = Simulation / modeling (Arienti, SNL)

CLSVOF simulations comparing BOB4 to x-ray experiment

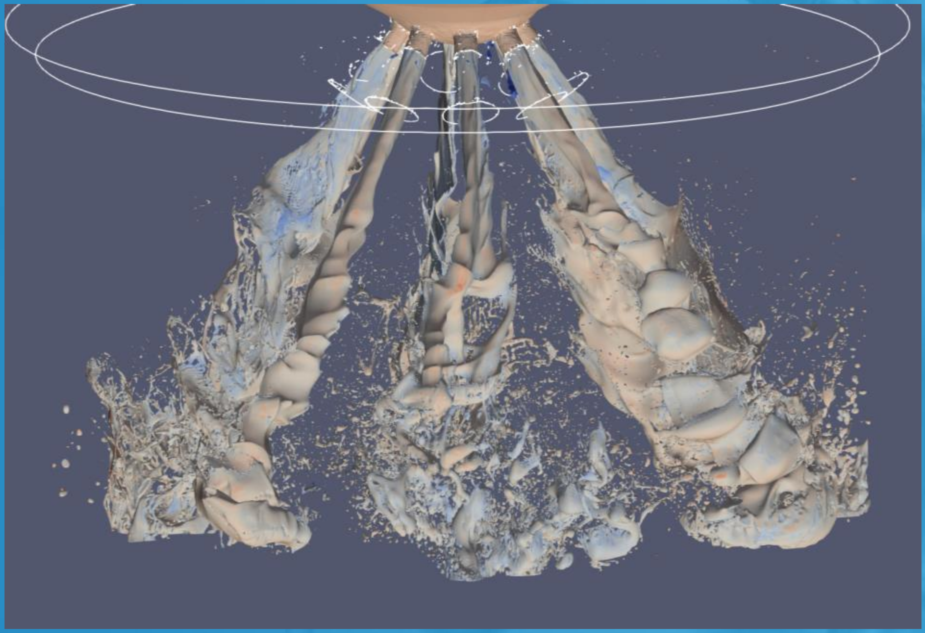
Boiling Point [°C]	Compound	Volume % for Surrogate BOB4
99.0	iso-octane	55
98.4	n-heptane	15
110.6	toluene	25
63.0	1-hexene	5

Spray G operating conditions (6 bar)



Profile from tangential average through plume center

- Spray G simulation with multiphase CLSVOF code for BOB4, mixture properties created using REFPROP library



Snapshot of partially-filled Spray G chamber during start of injection

Improving the homogenous relaxation model

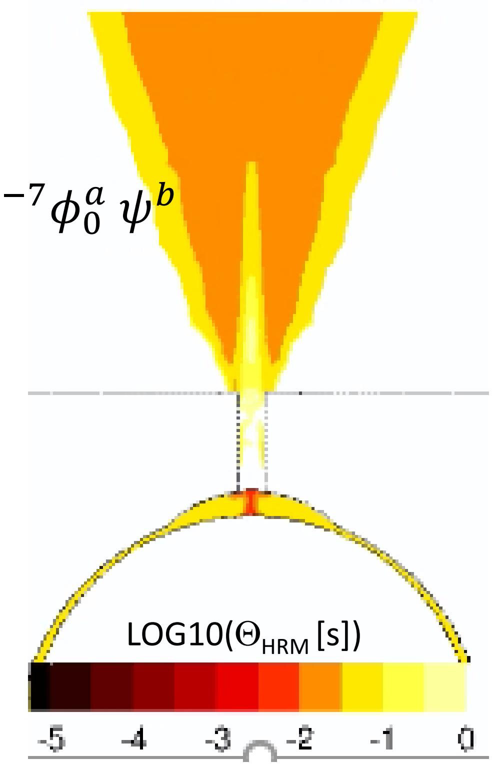
$$\frac{Dx}{Dt} = -\frac{x - \bar{x}}{\Theta_{HRM}}$$

Smaller Θ_{HRM} means faster relaxation to equilibrium

$$\Theta_{HRM} = 3.84 \cdot 10^{-7} \phi_0^a \, \psi^b$$

$$\psi = \left| \frac{P_{sat} - P}{P_{crit} - P_{sat}} \right|$$

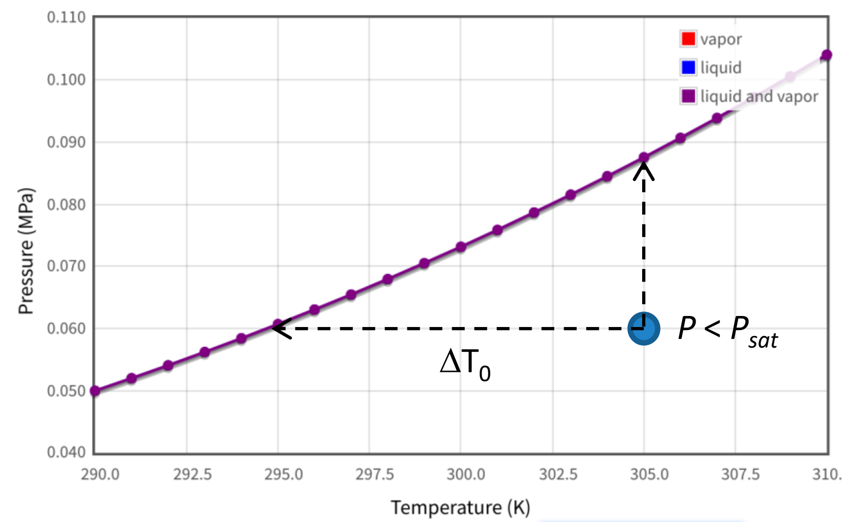
$$\phi_0 = \alpha \frac{n_{vap}}{n_{vap} + n_{N2}}$$



Single-hole simulations at flash-boiling conditions

New bubble submodel:

Pressure-temperature diagram at saturation



SM = Simulation / modeling (Arienti, SNL)

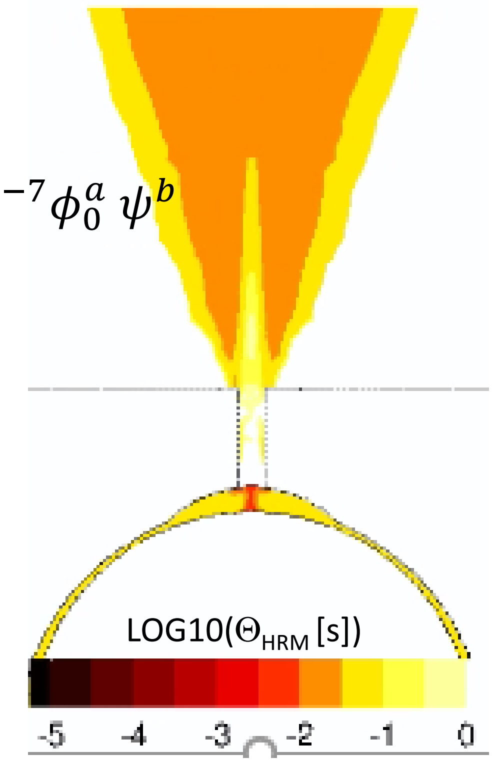
Consider bubble radius, position, temperature

$$\frac{Dx}{Dt} = -\frac{x-\overline{x}}{\Theta_{\mathrm{HRM}}}$$

$$\Theta_{\mathrm{HRM}} = 3.84 \cdot 10^{-7} \phi_0^a \, \psi^b$$

$$\psi = \left| \frac{P_{sat} - P}{P_{crit} - P_{sat}} \right|$$

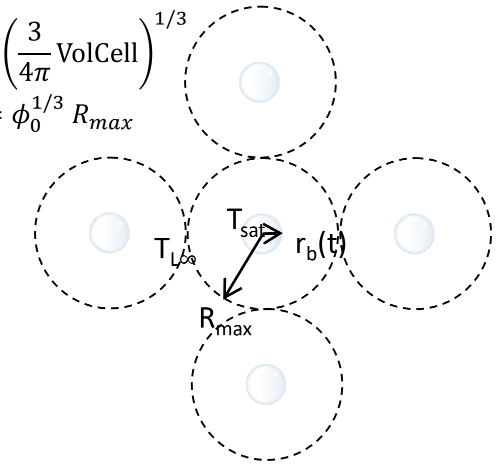
$$\phi_0 = \alpha \frac{n_{vap}}{n_{vap} + n_{N2}}$$



New bubble submodel:

$$R_{max} = \left(\frac{3}{4\pi}\mathrm{VolCell}\right)^{1/3}$$

$$r_b(0) = \phi_0^{1/3} R_{max}$$



$$\mathrm{Jac} = \frac{\rho_{vap}}{\rho_{liq}} \frac{c_{p,liq}\,\Delta T_0}{h_{vap}}$$

LOG10(Θ_{HRM} [s])

NEW: $\Theta_{\mathrm{HRM}}(\mathrm{Jac}, r_b(0))$

SM = Simulation / modeling (Arienti, SNL)

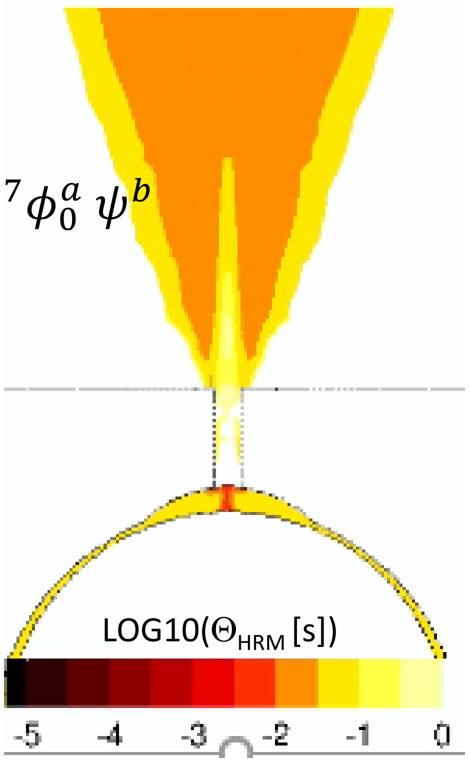
New model would have faster relaxation, faster vapor growth

$$\frac{\boldsymbol{Dx}}{\mathbf{D}\boldsymbol{t}} = -\frac{\boldsymbol{x} - \overline{\boldsymbol{x}}}{\boldsymbol{\Theta}_{\mathbf{HRM}}}$$

$$\Theta_{\mathrm{HRM}} = 3.84 \cdot 10^{-7} \phi_0^a \, \psi^b$$

$$\psi = \left|\frac{P_{sat} - P}{P_{crit} - P_{sat}}\right|$$

$$\phi_0 = \alpha \frac{n_{vap}}{n_{vap} + n_{N2}}$$



New bubble submodel:

Responses to Previous Year's Reviewers' Comments

General, Page 5-39: "The reviewer was pleased to see a focus on sprays, stated that there have been questions on how biofuels and other non-conventional fuels behave in sprays for decades. Once we understand the spray better, more effort can be put into the combustion systems."

OI	Page 5-39: "Many milestones were pending" but the new spray chamber capability is "good progress" because it is needed to be relevant to today's high-power density engines" • *The support is appreciated particularly because this project has made a substantial investment into a chamber for higher quality spray diagnostics for the future.*
XD	Page 5-41: "Using these diagnostics to dive into how these new fuel behave in sprays and what that does to mixture formation is fundamental and essential to the co-development of fuels and engines" • *The support is appreciated. We have tried to design this year's task with this goal in mind.*
SM	No reviewer comments; this project was a new start in FY18.

Collaboration and Coordination with Other Institutions

OI	• Sandia: using same fuel injection equipment as light-duty engine (Sjoberg) • Engine Combustion Network: data is being shared with ECN, several modeling groups are expected to contribute simulations for comparison with the measurements
XD	• Sandia: coordination with Pickett on measurement conditions • Engine Combustion Network: data is being shared with ECN, several modeling groups are expected to contribute simulations for comparison with the measurements
SM	• Engine Combustion Network: multiple investigators (~15) perform experiments and simulate the Spray G internal and external conditions used in these studies • Prof. Mark Sussman, Florida State Univ.: Development & testing of numerical methods for fuel inj. applications • Center for Computational Sciences & Engineering, Berkeley Lab: Development of library for hierarchical adaptive mesh refinement in high-performance computing

Remaining Challenges and Barriers

OI	• Liquid wall impingement is difficult to characterize but is closely linked to soot and PM emissions. Tailoring fuel delivery for multimode ignition/combustion requires precise control to maintain controlled flame while not forming PM.
XD	• Current measurements using x-ray radiography cannot resolve between liquid fuel and fuel vapor. X-ray fluorescence measurements are more challenging, but will allow us to quantify the liquid and vapor separately.
SM	• A major barrier is the high computational cost of a detailed fuel injection simulation, which limits how many operation points can be examined. The development of a data-driven process capable of integrating spray details in combustion simulations at the engine scale remains a substantial challenge.

Proposed Future Research

OI	• Quantify liquid penetration, plume direction and plume shape • Use high-pressure injection hardware specifically designed for short and multiple injection • High-speed long-distance microscopy for dribble at end of injection • Perform stratified-ignition experiments at relevant T and P
XD	• Droplet sizing using USAXS • Needle motion at flash-boiling conditions • Add’l measurements of flash-boiling GDI sprays using x-ray fluorescence
SM	• Simulation of liquid dribble at end of injection, with resulting ignition, combustion and soot formation • Implementation of more detailed computational models for cavitation and flash-boiling, in relation to the operation mode of modern injectors.

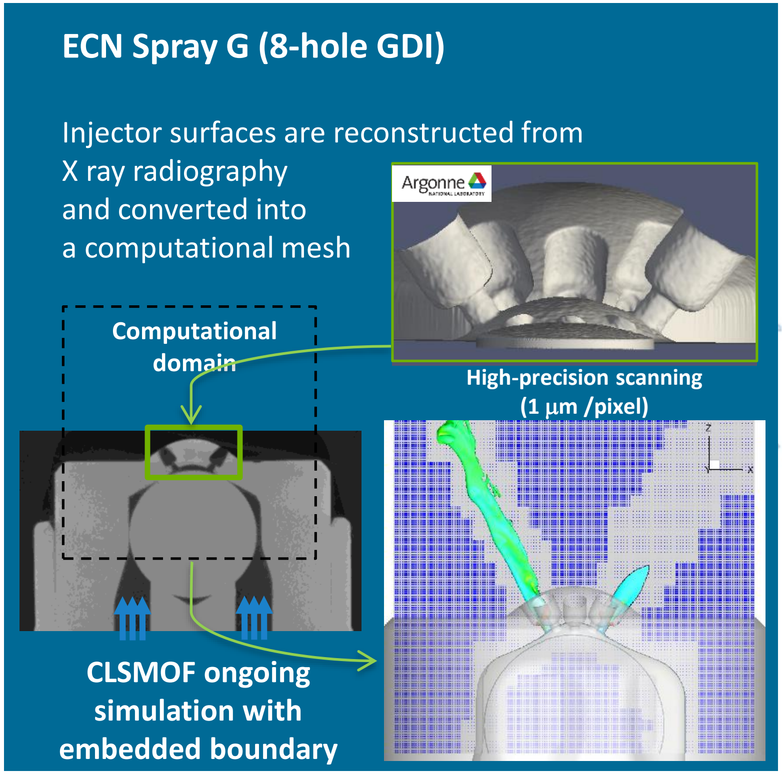
Summary

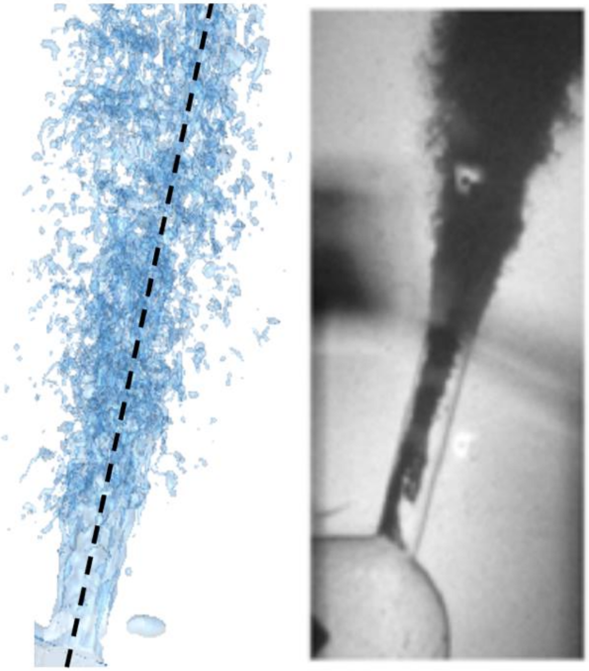
OI	• Showed major variation in spray mixing for leading-candidate fuels with a strong relationship on light distillate fraction (missing from current merit function) • Simultaneous ignition and flame propagation shown for mixed-mode conditions • Significant new diagnostic advancements for 3D plume direction
XD	• Near-nozzle fuel distributions have been measured for three fuel blends, several fuel temperatures, providing fundamental information about plume interaction and growth that is key for prediction of spray collapse
SM	• New homogenous relaxation model proposed/evaluated, showing potential to predict faster relaxation (more vaporization) at flash-boiling conditions

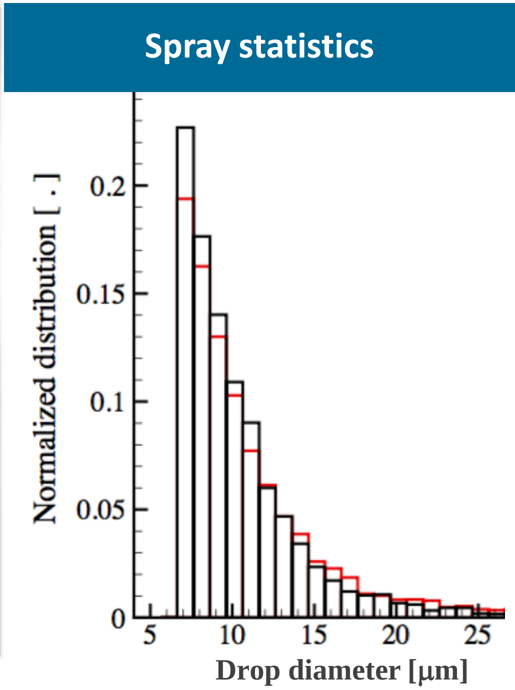
Technical Back-Up Slides

Computational Approach: The Multiphase Code CLSVOF

- Sharp-interface discretization of multi-phase Navier-Stokes eqns.
  - ✓Compressible effects
  - ✓Non-conformal, moving wall boundaries
  - ✓Adaptive mesh refinement
  - ✓Flexible EoS implementation







Increased scalability up to 900M cells (10,000 MPI processes on SNL and ANL platforms) with hybrid MPI / Open MP configuration.